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FILE COVERS 1967 - 31 Aug 1999 VOL 131 ISS 10
FILE LAST UPDATED: 31 Aug 1999 (19990831/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

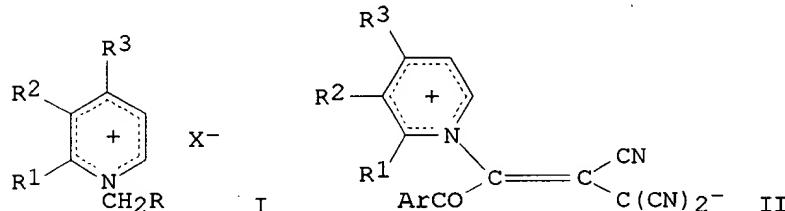
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=> s 11

L2 10 L1

=> d 1-10 iall

L2 ANSWER 1 OF 10 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1991:655361 CAPLUS
DOCUMENT NUMBER: 115:255361
TITLE: Regioselectivity of reactions of azinium salts and ylides with tetracyanoethylene
AUTHOR(S): Shestopalov, A. M.; Aitov, I. A.; Sharanin, Yu. A.; Litvinov, V. P.
CORPORATE SOURCE: Inst. Org. Khim. im. Zelinskogo, Moscow, USSR
SOURCE: Izv. Akad. Nauk SSSR, Ser. Khim. (1991), (6), 1431-9
CODEN: IASKA6; ISSN: 0002-3353
DOCUMENT TYPE: Journal
LANGUAGE: Russian
CLASSIFICATION: 22-4 (Physical Organic Chemistry)
OTHER SOURCE(S): CASREACT 115:255361
GRAPHIC IMAGE:



ABSTRACT:

Reaction of azinium salts I [R = e.g., H, COPh, CONH₂; R₁, R₂ = e.g., H, Me; (R₁R₂) = (CH:CH)₂; R₃ = H, Me; X = halide, ClO₄⁻] with TCNE in aq. MeOH at 20.degree. proceeded by hydrolysis/anion exchange, with formation of I [X = -OC(CN):C(CN)₂⁻]. Azinium ylides generated in the reaction of I (R = COAr, Ar = substituted Ph; R₁-R₃ = e.g., H, Me) with NET₃ in MeOH reacted with TCNE via a stereoselective addn.-elimination reaction, forming Z 1,4-ylides II. The mechanism of reaction was discussed.

SUPPL. TERM: TCNE stereoselective addn elimination azinium salt; ylide aroylpyridinotritycyanopropenide
INDEX TERM: Hydrolysis
(anion exchange and, in reaction of azinium salts with TCNE in aq. methanol)

INDEX TERM: Ylides
 ROLE: PRP (Properties)
 (aroylpyridinotricyanopropenides, stereoselective
 formation of, in reaction of azinium ylides with TCNE)

INDEX TERM: Addition reaction
 (stereoselective, elimination and, in reaction of
 azinium ylides with TCNE)

INDEX TERM: 930-73-4 3947-76-0 10129-51-8 41220-29-5 52805-99-9
 63008-23-1 78572-44-8 133828-84-9 136714-37-9
 136714-38-0
 ROLE: PRP (Properties)
 (anion exchange/hydrolysis reaction of, with TCNE)

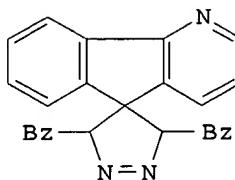
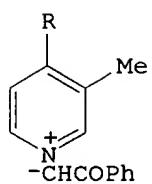
INDEX TERM: 16844-10-3 16883-69-5 32896-98-3
 ROLE: PRP (Properties)
 (anion exchange/hydrolysis reaction of, with TCNE, and
 stereoselective addn./elimination reaction of ylide
 derived from, with TCNE)

INDEX TERM: 670-54-2, TCNE, reactions
 ROLE: RCT (Reactant)
 (hydrolysis/anion exchange reaction of, with azinium
 salts, and stereoselective addn./elimination reaction
 of,
 with ylides derived from azinium salts)

INDEX TERM: 134720-91-5P 134720-92-6P 134720-95-9P 136714-39-1P
 136714-40-4P 136714-41-5P 136714-43-7P 136714-44-8P
 136714-46-0P 136714-48-2P 136714-50-6P 136714-51-7P
 136714-53-9P 136714-54-0P 136714-57-3P 136714-58-4P
 136714-59-5P 136714-60-8P 136714-61-9P 136714-62-0P
 136714-63-1P 136714-64-2P 136714-65-3P 136714-66-4P
 136974-27-1P
 ROLE: SPN (Synthetic preparation); PREP (Preparation)
 (prep. of)

INDEX TERM: 7250-28-4 17282-37-0 25357-43-1 26031-66-3
 82746-41-6 82746-43-8 136106-08-6 136714-55-1
 136714-56-2
 ROLE: PRP (Properties)
 (stereoselective addn./elimination reaction of ylide
 derived from, with TCNE)

L2 ANSWER 2 OF 10 CAPLUS COPYRIGHT 1999 ACS
 ACCESSION NUMBER: 1990:478234 CAPLUS
 DOCUMENT NUMBER: 113:78234
 TITLE: New method of 1-pyrazoline ring formation
 AUTHOR(S): Prostakov, N. S.; Varlamov, A. V.; Annan, Hussein;
 Fomichev, A. A.; Aliev, A. E.
 CORPORATE SOURCE: Univ. Druzhby Nar. im. P. Lumumby, Moscow, 117923,
 USSR
 SOURCE: Khim. Geterotsikl. Soedin. (1989), (12), 1697
 CODEN: KGSSAQ; ISSN: 0453-8234
 DOCUMENT TYPE: Journal
 LANGUAGE: Russian
 CLASSIFICATION: 28-8 (Heterocyclic Compounds (More Than One Hetero
 Atom))
 OTHER SOURCE(S): CASREACT 113:78234
 GRAPHIC IMAGE:



ABSTRACT:

Treating ylides I (R = Ph₃Si, H), generated from the corresponding N-phenacylpyridinium bromides by aq. K₂CO₃ in CHCl₃ at 20.°, with 9-diazo-4-azafluorene in CHCl₃ for 5 h at 20.°, gave 35 and 32% spiropyrazoline deriv. II.

SUPPL. TERM: phenacylpyridinium ylide diazotization cyclization;
INDEX TERM: spirocarbazolepyrazole; pyrazole spirocarbazole
INDEX TERM: Ring closure and formation
INDEX TERM: (of phenacylpyridine ylides with diazoazafluorene,
INDEX TERM: spiro[azafluorene-pyrazoline] derivs. from)
INDEX TERM: Ylides
INDEX TERM: ROLE: RCT (Reactant)
INDEX TERM: (of phenacylpyridines, cyclization by diazoazafluorene)
INDEX TERM: Spiro compounds
INDEX TERM: ROLE: SPN (Synthetic preparation); PREP (Preparation)
INDEX TERM: (prepn. of spiro[azafluorene-pyrazoline] deriv.)
INDEX TERM: 50555-86-7
INDEX TERM: ROLE: RCT (Reactant)
INDEX TERM: (cyclization by, of phenacylpyridine ylides,
INDEX TERM: spiro[azafluorene-pyrazoline] derivs. from)
INDEX TERM: 56241-32-8 67433-80-1
INDEX TERM: ROLE: RCT (Reactant)
INDEX TERM: (cyclization of, by diazoazafluorene,
INDEX TERM: spiro[azafluorene-pyrazoline] deriv. from)
INDEX TERM: 16844-10-3 67433-79-8
INDEX TERM: ROLE: RCT (Reactant)
INDEX TERM: (generation of ylide from)
INDEX TERM: 128381-32-8P 128443-23-2P
INDEX TERM: ROLE: SPN (Synthetic preparation); PREP (Preparation)
INDEX TERM: (prepn. of)

L2 ANSWER 3 OF 10 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1986:590862 CAPLUS
 DOCUMENT NUMBER: 105:190862
 TITLE: Stereochemical study on 1,3-dipolar cycloaddition
 reactions of heteroaromatic N-ylides with
 symmetrically substituted cis and trans olefins
 AUTHOR(S): Tsuge, Otohiko; Kanemasa, Shuji; Takenaka, Shigeori
 CORPORATE SOURCE: Interdiscip. Grad. Sch. Eng. Sci., Kyushu Univ.,
 Kasuga, 816, Japan
 SOURCE: Bull. Chem. Soc. Jpn. (1985), 58(11), 3137-57
 CODEN: BCSJA8; ISSN: 0009-2673
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 CLASSIFICATION: 27-16 (Heterocyclic Compounds (One Hetero Atom))
 OTHER SOURCE(S): CASREACT 105:190862

ABSTRACT:

Stereochem. of the cycloaddns. of twenty-four heteroarom. N-ylides with sym. substituted cis and trans olefins has been investigated. Cyclic and acyclic cis olefins cycloadd to the anti form of the ylides in a highly endo-selective manner giving almost quant. yields of stereospecific endo 3+2 cycloadducts. N-Ylides stabilized with a substituent of the carbonyl type react with trans

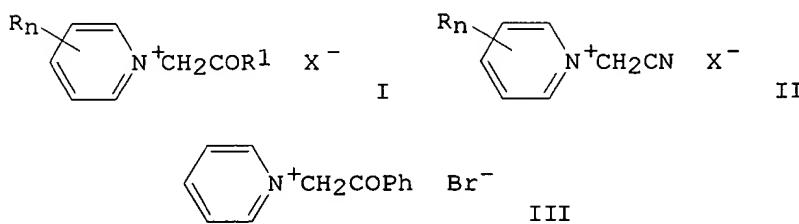
olefins to form mostly 2 stereoisomeric 3+2 cycloadducts to the anti form of the ylides. In most cases, they undergo stereospecific interconversion through a retro cycloaddn. process, the isomer ratios and the ease of transformation depending upon the nature and size of substituents on the 5-membered ring which has been built up in the cycloaddn. step. On the other hand, N-ylides stabilized with a substituent of noncarbonyl type react with trans olefins to give stereospecific and stereoselective 3+2 cycloadducts as single isomers which are assigned as the cycloadducts to the syn form of the ylides.

SUPPL. TERM: ylide heteroarom olefin cycloaddn stereochem
 INDEX TERM: Cycloalkenes
 Alkenes, reactions
 ROLE: RCT (Reactant)
 (cycloaddn. of, with heteroarom. N-ylides, stereochem.
 of)
 INDEX TERM: Ylides
 ROLE: RCT (Reactant)
 (heteroarom. N-, cycloaddn. of, with olefins,
 stereochem.
 of)
 INDEX TERM: Stereochemistry
 (of cycloaddn. of heteroarom. N-ylides with olefins)
 INDEX TERM: Cycloaddition reaction
 (of heteroarom. N-ylides with olefins, stereochem. of)
 INDEX TERM: 762-42-5
 ROLE: PROC (Process)
 (addn. of, with diazatricyclododecadienes)
 INDEX TERM: 624-48-6 624-49-7 764-42-1 928-53-0 930-88-1
 941-69-5 959-27-3 959-28-4 1081-17-0 1631-28-3
 2973-17-3 7633-38-7 18305-60-7
 ROLE: PROC (Process)
 (cycloaddn. of, with heteroarom. N-ylides, stereochem.
 of)
 INDEX TERM: 108-31-6, reactions
 ROLE: RCT (Reactant)
 (cycloaddn. of, with heteroarom. N-ylides, stereochem.
 of)
 INDEX TERM: 289-80-5 946-07-6 4329-73-1 5304-34-7 7250-28-4
 7467-00-7 16726-82-2 **16844-10-3** 16883-69-5
 17282-40-5 17282-41-6 17282-43-8 18667-21-5
 25131-60-6 25357-39-5 25357-50-0 25357-51-1
 26489-32-7 32896-98-3 33014-32-3 39595-94-3
 40448-79-1 40448-80-4 51386-37-9 55814-00-1
 55841-58-2 56241-32-8 56567-29-4 57699-26-0
 58329-45-6 59456-80-3 59986-29-7 64636-81-3
 72797-44-5 72797-45-6 78113-64-1 80636-51-7
 82735-58-8 87773-11-3 88089-35-4 88089-43-4
 88089-46-7 90625-75-5 92171-46-5 104932-95-8
 104932-96-9 104932-97-0 104953-23-3 104953-24-4
 ROLE: PROC (Process)
 (cycloaddn. of, with olefins, stereochem. of)
 INDEX TERM: 104953-21-1P
 ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation)
 (prepn. and oxidn. of)
 INDEX TERM: 37129-40-1P 78113-52-7P 78113-53-8P 78113-54-9P
 78184-05-1P 78184-06-2P 78184-07-3P 88089-36-5P
 88089-37-6P 88089-38-7P 88089-39-8P 88089-40-1P
 88089-41-2P 88089-44-5P 88089-45-6P 88121-62-4P
 88121-63-5P 90625-67-5P 90625-68-6P 90625-69-7P
 90625-70-0P 90625-71-1P 90625-72-2P 90625-73-3P

90625-74-4P	90650-46-7P	90650-47-8P	97204-08-5P
97204-09-6P	97204-10-9P	97204-11-0P	97204-12-1P
97204-13-2P	97204-14-3P	97204-15-4P	97226-60-3P
97275-41-7P	97275-42-8P	97275-43-9P	97275-44-0P
104932-92-5P	104932-93-6P	104932-94-7P	104932-99-2P
104933-00-8P	104933-01-9P	104953-14-2P	104953-15-3P
104953-16-4P	104953-17-5P	104953-18-6P	104953-19-7P
104953-20-0P	104953-22-2P	104953-25-5P	104953-26-6P
104953-27-7P	104953-28-8P	104953-29-9P	104953-30-2P
105016-33-9P	105017-09-2P	105017-10-5P	105017-11-6P
105017-12-7P	105017-13-8P	105017-14-9P	105017-15-0P
105017-16-1P	105017-17-2P	105017-18-3P	105017-19-4P
105017-20-7P			
ROLE: SPN (Synthetic preparation); PREP (Preparation)			
(prep. of)			
INDEX TERM:	100-48-1	110-86-1, reactions	119-65-3 288-47-1
	591-22-0	3796-23-4	
	ROLE: RCT (Reactant)		
	(quaternization of)		
INDEX TERM:	70-11-1	590-17-0	2114-00-3 15109-94-1
	ROLE: RCT (Reactant)		
	(reaction of, with pyridine)		

L2 ANSWER 4 OF 10 CAPLUS COPYRIGHT 1999 ACS
 ACCESSION NUMBER: 1981:165607 CAPLUS
 DOCUMENT NUMBER: 94:165607
 TITLE: Pyridinium compound fogging agents for photographic material
 INVENTOR(S): Oishi, Yasushi; Hirano, Shigeo
 PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
 SOURCE: Ger. Offen., 70 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 INT. PATENT CLASSIF.: G03C005-30
 CLASSIFICATION: 74-2 (Radiation Chemistry, Photochemistry, and Photographic Processes)
 Section cross-reference(s): 27
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3014628	A1	19801030	DE 1980-3014628	19800416
DE 3014628	C2	19910502		
JP 55138742	A2	19801029	JP 1979-46949	19790417
JP 62004699	B4	19870131		
US 4324855	A	19820413	US 1980-140923	19800416
PRIORITY APPLN. INFO.:			JP 1979-46949	19790417
GRAPHIC IMAGE:				



ABSTRACT:

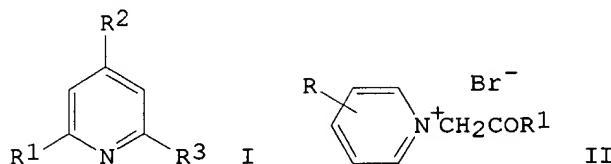
Reversal images with a higher Dmax and a lower Dmin can be produced by incorporation of nucleating agents (fogging agents) of the formulas I or II (R = trihalomethyl, CN, carbamoyl, a carboxyl ester, carboxamido, sulfonamido, acyl, sulfonyl, sulfamoyl, acylamino, aryl, alkyl, or heterocycle; R1 = a mono-, di-, or tricyclic aryl group, a heterocycle, or a straight chain, branched chain, or cyclic alkyl; X- = anion; n = 0-3) into an internal latent image-forming emulsion layer contg. a dye-forming compd. and subsequently processing with an alk. soln. after imagewise exposure. Thus, a transparent cellulose acetate film support was coated with a layer contg. a magenta dye-releasing redox compd., a layer of a spectrally sensitized internal latent image-forming gelatin-AgBr emulsion contg. III 1.4 mmol/mol Ag, and a protective gelatin layer. This unit was then exposed, combined with a receptor element contg. a mordant, and processed with an alk. processing soln. to give a magenta pos. image with a Dmin of 0.03 and a Dmax of 1.25.

SUPPL. TERM: cyanoethylpyridinium fogging agent photog;
aroylethylpyridinium fogging agent photog;
alkanoylmethylpyridinium fogging agent photog; pyridinium deriv fogging agent photog; nucleating agent pyridinium deriv photog
INDEX TERM: 5469-10-3 6277-72-1 6299-99-6 **16844-10-3**
16844-14-7 16883-69-5 17281-59-3 17282-37-0
17282-38-1 25357-39-5 25357-44-2 25357-46-4
25407-31-2 26031-47-0 26031-59-4 26031-66-3
26535-84-2 42508-60-1 49854-35-5 63374-35-6
64881-07-8 69656-16-2 77281-09-5 77281-10-8
77281-11-9 77281-12-0 77281-13-1 77281-14-2
77281-15-3 77281-16-4 77281-17-5 77281-18-6
77281-19-7 77281-20-0 77281-21-1 77281-22-2
77281-23-3 77281-24-4 77281-25-5 77281-26-6
77281-27-7 77281-28-8 77281-29-9 77281-30-2
77281-31-3 77281-32-4 77281-33-5 77281-34-6
77281-35-7
ROLE: USES (Uses)
(photog. fogging agent, for reversal image prodn.)
INDEX TERM: 29536-25-2P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of, with phenacyl bromide)
INDEX TERM: 20260-53-1
ROLE: RCT (Reactant)
(reaction of, with cetylamine)
INDEX TERM: 143-27-1
ROLE: RCT (Reactant)
(reaction of, with nicotinoyl chloride hydrochloride)
INDEX TERM: 70-11-1
ROLE: RCT (Reactant)
(reaction of, with N-hexadecylnicotinamide)

L2 ANSWER 5 OF 10 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1981:65440 CAPLUS
DOCUMENT NUMBER: 94:65440
TITLE: Studies on cycloimmonium ylides. Synthesis of some 2,4,6-triaryl-substituted pyridines via picolinium ylides
AUTHOR(S): Tewari, Ram. S.; Dubey, Ajay K.; Misra, Naresh K.; Dixit, Priya D.
CORPORATE SOURCE: Dep. Chem., H. B. Technol. Inst., Kanpur, 208002, India

SOURCE: J. Chem. Eng. Data (1981), 26(1), 106-8
DOCUMENT TYPE: CODEN: JCEAAZ; ISSN: 0021-9568
LANGUAGE: Journal
CLASSIFICATION: English
GRAPHIC IMAGE: 27-17 (Heterocyclic Compounds (One Hetero Atom))



ABSTRACT:

2,4,6-Triaryl-substituted pyridines I were prepd. by reaction of aroylmethylenepicolinium ylides II ($R = 3\text{-Me, 4\text{-Me; } R1 = Ph, 4\text{-ClC}_6\text{H}_4, p\text{-tolyl)}$) with $R2\text{CH:CHCOR3}$ ($R2, R3 = \text{optionally substituted Ph}$).

SUPPL. TERM: pyridine triphenyl; cyclocondensation picolinium ylide
 chalcone
 INDEX TERM: Cyclocondensation reaction
 (of picolinium ylides with chalcones, substituted
 pyridines from)
 INDEX TERM: 94-41-7 959-23-9 1230-77-9 2373-89-9 2453-44-3
 5416-71-7 6552-63-2 6552-66-5 6552-68-7 19133-00-7
 19672-59-4 21551-47-3 42580-60-9 69538-64-3
 72666-54-7 73911-01-0 75573-20-5 75573-21-6
 ROLE: RCT (Reactant)
 (cyclocondensation of, with picolinium ylides,
 substituted pyridine from)
 INDEX TERM: 16844-10-3 25357-43-1 76337-69-4
 ROLE: RCT (Reactant)
 (cyclocondensation of, with substituted chalcones,
 substituted pyridine from)
 INDEX TERM: 580-35-8P 3557-65-1P 16112-42-8P 72666-41-2P
 72666-42-3P 72666-45-6P 72666-47-8P 72666-48-9P
 72666-49-0P 72666-50-3P 72673-14-4P 73910-87-9P
 73910-89-1P 75573-10-3P 75573-11-4P 75573-12-5P
 75573-13-6P 75573-14-7P 75573-15-8P
 ROLE: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

L2 ANSWER 6 OF 10 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1978:22552 CAPLUS

DOCUMENT NUMBER: 88:22552

TITLE: Reaction of pyridinium N-ylides with ketene

thioacetal

derivatives

AUTHOR(S): Tominaga, Yoshinori; Miyake, Yoshinori; Fujito, Hiroshi; Kurata, Keiji; Awaya, Hiroyoshi; Matsuda, Yoshiro; Kobayashi, Goro

CORPORATE SOURCE: Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, Japan
SOURCE: Chem. Pharm. Bull. (1977), 25(7), 1528-33

CODEN: CPBTAL

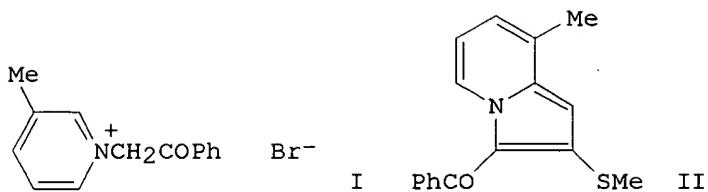
DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 27-17 (Hetero)

GRAPHIC IMAGE:

CHARGE TRICE.

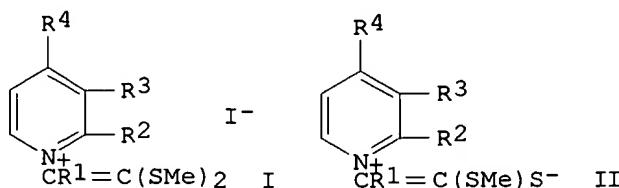


ABSTRACT:

Reaction of the pyridinium N-ylides with ketenethioacetal in the presence of Et₃N or K₂CO₃ as a base in EtOH or DMF gave the pyridinium N-allylides which readily cyclized to give the indolizine derivs. Thus, the pyridinium ylide I and (MeS)₂C:CHNO₂ gave the indolizine II.

SUPPL. TERM: pyridinium ylide reaction ketenethioacetal; indolizine
 INDEX TERM: Cyclocondensation reaction
 (of methylpyridinium ylides with ketene thioacetal
 derivs., indolizine derivs. from)
 INDEX TERM: Ylides
 ROLE: RCT (Reactant)
 (pyridinium, reaction of, with ketene thioacetal
 derivs.)
 INDEX TERM: 57845-14-4P 57845-15-5P 59182-01-3P 64908-40-3P
 64908-43-6P 64995-24-0P 64995-25-1P 64995-26-2P
 64995-27-3P 64995-28-4P 64995-29-5P 64995-30-8P
 64995-31-9P 64995-32-0P 64995-33-1P 64995-34-2P
 64995-35-3P 64995-36-4P 64995-37-5P 64995-38-6P
 ROLE: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)
 INDEX TERM: 7250-28-4 16844-10-3 16883-69-5 17282-40-5
 41220-29-5 56567-29-4 64636-79-9 64636-80-2
 64995-39-7 64995-40-0 64995-41-1 64995-42-2
 64995-43-3
 ROLE: RCT (Reactant)
 (reaction of, with ketenethioacetals)
 INDEX TERM: 3490-92-4 5147-80-8 13623-94-4 17823-58-4
 18374-66-8
 ROLE: RCT (Reactant)
 (reaction of, with pyridinium ylides)

L2 ANSWER 7 OF 10 CAPLUS COPYRIGHT 1999 ACS
ACCESSION NUMBER: 1977:601268 CAPLUS
DOCUMENT NUMBER: 87:201268
TITLE: Heterocyclic ketene thioacetal derivatives. VIII.
Synthesis of ketene thioacetals having a pyridinium salt
AUTHOR(S): Tominaga, Yoshinori; Miyake, Yoshinori; Fujito, Hiroshi; Matsuda, Yoshiro; Kobayashi, Goro
CORPORATE SOURCE: Fac. Pharm. Sci., Nagasaki Univ., Nagasaki, Japan
SOURCE: Yakugaku Zasshi (1977), 97(8), 927-32
CODEN: YKKZAJ
DOCUMENT TYPE: Journal
LANGUAGE: Japanese
CLASSIFICATION: 27-17 (Heterocyclic Compounds (One Hetero Atom))
GRAPHIC IMAGE:



ABSTRACT:

Ketenethioacetal derivs. I (R1 = Bz, CO2Et, CONH2, CN; R2, R3, R4 = H, Me) were prep'd. by alkylation with MeI of II, which were prep'd. by the reaction of pyridinium ylides with CS2 in the presence o NaOH.

SUPPL. TERM: pyridinium ketene thioacetal deriv; ylide pyridinium reaction carbon disulfide

INDEX TERM: Mercaptals and Mercaptoles

ROLE: RCT (Reactant)
(ketene thioacetals with a pyridinium salt)

INDEX TERM: Ylides

ROLE: RCT (Reactant)
(pyridinium, reaction of, with carbon disulfide)

INDEX TERM: 64636-63-1P 64636-64-2P 64636-65-3P 64636-66-4P
64636-67-5P 64636-68-6P 64636-69-7P 64636-70-0P
64636-71-1P 64636-72-2P 64636-73-3P 64636-74-4P

ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction with methyl iodide)

INDEX TERM: 57845-27-9P 59181-92-9P 59181-93-0P 59181-94-1P
59181-95-2P 59181-96-3P 59181-97-4P 59181-98-5P
64636-75-5P 64636-76-6P 64636-82-4P 64636-83-5P

ROLE: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

INDEX TERM: 7250-28-4 **16844-10-3** 17282-40-5 26557-57-3
32896-98-3 42866-67-1 55814-02-3 64636-77-7
64636-78-8 64636-79-9 64636-80-2 64636-81-3

ROLE: RCT (Reactant)
(reaction of, with carbon disulfide and dimethyl sulfate)

INDEX TERM: 75-15-0, reactions

ROLE: RCT (Reactant)
(reaction of, with pyridinium ylides)

INDEX TERM: 74-88-4, reactions 75-18-3

ROLE: RCT (Reactant)
(reaction of, with sulfur contg. pyridinium ylides)

L2 ANSWER 8 OF 10 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1975:514165 CAPLUS

DOCUMENT NUMBER: 83:114165

TITLE: Route to 2,6-dihydroxypiperidines

AUTHOR(S): Wild, Peter; Kroehnke, Fritz

CORPORATE SOURCE: Inst. Org. Chem., Univ. Giessen, Giessen, Ger.

SOURCE: Justus Liebigs Ann. Chem. (1975), (5), 849-63

CODEN: JLACBF

DOCUMENT TYPE: Journal

LANGUAGE: German

CLASSIFICATION: 27-17 (Heterocyclic Compounds (One Hetero Atom))

GRAPHIC IMAGE: For diagram(s), see printed CA Issue.

ABSTRACT:

Acylalkylpyridinium salts I (R = H, 3-Me, 4-Me, 3,5-Me2; R1 = Me, Ph, 4-MeC6H4)

reacted with R₂CHO (R₂ = H, Ph, 4-MeC₆H₄) and R₃NH₂ (R₃ = H, Me) in a 2:1:1 molar ratio to give .apprx.60% dipyridinium salts II. II lost 1 mole H₂O to give tetrahydro derivs. III and a 2nd mole H₂O to give dihydro derivs. IV. IV were dehydrogenated to the corresponding pyridine compds. which were readily ring-cleaved to give pyridinediamines V and glutaconaldehyde deriv. VI. Excess piperidine causes chain-shortening of VI.

SUPPL. TERM: acylpyridinium reaction aldehyde ammonia; pyridinium acyl reaction aldehyde ammonia; amine reaction acylpyridinium; hydroxypiperidinediylidypyridinium; piperidinediylidypyridinium dihydroxy; glutaconaldehyde Schiff base; dehydration dihydroxypiperidinediylidypyridinium

INDEX TERM: Dehydration, chemical (acid-catalyzed, of (dihydroxypiperidinediyl)dipyridinium salts)

INDEX TERM: Aldehydes, reactions

ROLE: RCT (Reactant) (with acylalkylpyridinium salts and ammonia)

INDEX TERM: 56566-74-6P 56566-75-7P 56566-76-8P 56566-77-9P
56566-78-0P 56566-81-5P 56566-82-6P 56566-83-7P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and dehydration of)

INDEX TERM: 56566-87-1P 56566-89-3P 56566-91-7P 56566-93-9P
56566-97-3P 56567-05-6P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and dehydrogenation of)

INDEX TERM: 56567-15-8P 56567-17-0P 56567-19-2P 56567-21-6P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and ring cleavage of)

INDEX TERM: 2473-39-4P 2473-40-7P 56566-80-4P 56566-85-9P
56566-95-1P 56566-99-5P 56567-01-2P 56567-03-4P
56567-07-8P 56567-09-0P 56567-11-4P 56567-13-6P
56567-23-8P 56567-25-0P 56567-26-1P 56567-27-2P
56567-28-3P 56567-30-7P 56567-31-8P 56567-32-9P
56567-34-1P 56567-36-3P
ROLE: SPN (Synthetic preparation); PREP (Preparation) (prepn. of)

INDEX TERM: 16883-69-5
ROLE: RCT (Reactant) (reaction with aldehydes and ammonia or methylamine)

INDEX TERM: 7250-28-4 **16844-10-3** 56567-29-4
ROLE: RCT (Reactant) (reaction with benzaldehyde and ammonia)

INDEX TERM: 17282-38-1 17282-41-6
ROLE: RCT (Reactant) (reaction with methylbenzaldehyde and ammonia)

INDEX TERM: 104-87-0
ROLE: RCT (Reactant) (reaction with phenacyl- or acetylpyridinium bromides and ammonia)

INDEX TERM: 74-89-5
ROLE: RCT (Reactant) (reaction with phenacylpyridinium bromide and benzaldehyde)

INDEX TERM: 7664-41-7, reactions
ROLE: RCT (Reactant) (with phenacyl- or acetylpyridinium bromides and

INDEX TERM: aldehydes)
 100-52-7, reactions
 ROLE: RCT (Reactant)
 (with phenacyl- or acetylpyridinium bromides and
 ammonia or methylamine)
 INDEX TERM: 50-00-0, reactions
 ROLE: RCT (Reactant)
 (with phenacylpyridinium bromide and ammonia)

 L2 ANSWER 9 OF 10 CAPLUS COPYRIGHT 1999 ACS
 ACCESSION NUMBER: 1974:36969 CAPLUS
 DOCUMENT NUMBER: 80:36969
 TITLE: Synthesis and thermal reaction of pyridinium
 3,3-diacyl-1-benzoylallylides[3,3-diacyl-1-benzoyl-1-
 (1-pyridinio)prop-2-enides]. Formation of indolizine
 derivatives
 AUTHOR(S): Tamura, Yasumitsu; Sumida, Yoshio; Ikeda, Masazumi
 CORPORATE SOURCE: Fac. Pharm. Sci., Osaka Univ., Osaka, Japan
 SOURCE: J. Chem. Soc., Perkin Trans. 1 (1973), (19), 2091-5
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 CLASSIFICATION: 27-17 (Heterocyclic Compounds (One Hetero Atom))
 GRAPHIC IMAGE: For diagram(s), see printed CA Issue.
 ABSTRACT:
 Pyridinium phenacylides with 2,2-diacyl-1-ethoxyethylenes gave pyridinium
 3,3-diacyl-1-benzoyl-allylides. E.g. pyridinium phenacylide with
 $\text{EtOCH}_2\text{C}(\text{COMe})_2$ gave 75% allylide (I, R = H). I (R = H) in refluxing $\text{Me}_2\text{C}_6\text{H}_4$
 gave 6% indolizine (II; R = H, R1 = Bz). 2-Methyl derivs. of I in refluxing
 $\text{Me}_2\text{C}_6\text{H}_4$ gave mainly 1-acetyl-2-phenylindolizines. E.g. I (R = Me) gave 30% II
(R = Ph, R1 = CH:CHCOMe) and 2% II (R = H, R1 = Bz).

 SUPPL. TERM: pyridinium allylide; pyridiniopropenide; propenide
 INDEX TERM: pyridinio; cyclization pyridinium allylide indolizine
 Ring closure and formation
 (of pyridinium diacylbenzoylallylides, indolizines by)
 INDEX TERM: 70-11-1
 ROLE: PROC (Process)
 (cycloaddn. of, with acetylpyridine)
 INDEX TERM: 7250-28-4 16844-10-3 16883-69-5
 ROLE: PROC (Process)
 (cycloaddn. of, with acetylacetylene)
 INDEX TERM: 6302-02-9
 ROLE: PROC (Process)
 (cycloaddn. of, with phenacyl bromide)
 INDEX TERM: 1423-60-5
 ROLE: PROC (Process)
 (cycloaddn. of, with phenacylpyridinium bromide)
 INDEX TERM: 51386-31-3P 51386-32-4P 51386-33-5P 51386-34-6P
 51386-35-7P 51386-36-8P 51386-40-4P 51386-41-5P
 51386-42-6P 51386-43-7P 51386-44-8P 51386-45-9P
 51386-46-0P 51386-47-1P 51386-48-2P 51386-49-3P
 ROLE: SPN (Synthetic preparation); PREP (Preparation)
 (prep. of)
 INDEX TERM: 17282-43-8 25357-50-0 51386-37-9 51386-38-0
 51386-39-1
 ROLE: RCT (Reactant)
 (reaction of, with (ethoxymethylene)pentanedione)
 INDEX TERM: 87-13-8 94-05-3 33884-41-2
 ROLE: RCT (Reactant)
 (reaction of, with pyridinium phenacylides)

L2 ANSWER 10 OF 10 CAPLUS COPYRIGHT 1999 ACS

ACCESSION NUMBER: 1967:453263 CAPLUS
DOCUMENT NUMBER: 67:53263
TITLE: Kinetics of the reaction of pyridines with phenacyl bromide in nitrobenzene
AUTHOR(S): Litvinenko, L. M.; Perel'man, L. A.
CORPORATE SOURCE: Donetsk. Gos. Univ., Donetsk, USSR
SOURCE: Zh. Org. Khim. (1967), 3(5), 936-42
CODEN: ZORKAE
DOCUMENT TYPE: Journal
LANGUAGE: Russian
CLASSIFICATION: 22 (Physical Organic Chemistry)

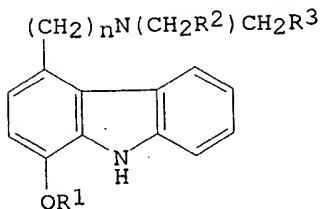
ABSTRACT:

The title reaction was found to proceed irreversibly and nearly quant. with formation of compds. of general formula $(RC_5H_4N+CH_2Bz)Br^-$ (I), where RC_5H_4N is substituted pyridine. The reaction kinetics were followed by potentiometric titrn. of the appearing Br^- . Rate consts. (k), activation energies (E), entropy changes (ΔS), and log A (A frequency factor) were calcd. Also Hammett-Taft consts., σ_0 and ρ_0 , were detd. from the equation $\log KR - \log KH = \rho_0 \sigma_0$ (R , m.p., σ , ΔS , K at 25. $^\circ$ C, K at 40. $^\circ$ C, K at 55. $^\circ$ C in 1. mole-1 sec.-1 times. 103, E in cal. mole-1, S in cal. degree-1 mole-1, log A in 1. mol.-1 sec.-1 given) H , 206.5. $^\circ$ C, 0, 1.93 \pm 0.04, 4.80 \pm 0.16, 12.6 \pm 0.5, 11,900, -33.8, 6.01; 3-Me, 189-90. $^\circ$ C, -0.07, 4.84 \pm 0.03, 10.2 \pm 0.2, 22.9 \pm 0.7, 11,000, -34.5, 5.65; 3-NO₂, 201-2. $^\circ$ C, 0.70, 0.00338 \pm 0.00014, 0.0104 \pm 0.0001, 0.0289 \pm 0.0002, 13,900, -39.7, 4.73; 3-Br, 194-5. $^\circ$ C, 0.38, 0.0660 \pm 0.0011, 0.185 \pm 0.008, 0.472 \pm 0.010, 12,800, -37.6, 5.18; 4-Et, 218-19. $^\circ$ C, -0.15, 5.83 \pm 0.14, 15.2 \pm 0.7, 32.0 \pm 0.8, 11,100, -34.3, 5.89; 4-NH₂, 299-300. $^\circ$ C, -0.38, 179.0 \pm 0.6, 378.0 \pm 17.0, 729.0 \pm 25.0, 9100, -34.1, 5.95; 3-Bz, 238-40. $^\circ$ C, 0.34, 0.170 \pm 0.003, -, -, -, -, 4-Ph, 203-5. $^\circ$ C, 0, 2.63 \pm 0.13, 6.55 \pm 0.10, 14.8 \pm 0.7, 11,200, -35.5, 5.64.

SUPPL. TERM: HAMMETT TAFT KINETICS; PHENACYL BROMIDE PYRIDINES KINETICS;
PYRIDINES KINETICS PHENACYL BROMIDE
INDEX TERM: Activation energy
Frequency factor
(of 2-bromoacetophenone reaction with pyridines)
INDEX TERM: Kinetics, reaction
(of 2-bromoacetophenones with pyridines)
INDEX TERM: Entropy
(of activation, of 2-bromoacetophenone reaction with pyridines)
INDEX TERM: 6299-99-6P 16844-10-3P 16844-11-4P 16844-13-6P
16844-14-7P 16844-15-8P 16883-69-5P 16883-70-8P
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(prep. of)
INDEX TERM: 108-99-6 504-24-5 536-75-4 626-55-1 939-23-1
2530-26-9 5424-19-1
ROLE: PRP (Properties)
(reaction with 2-bromoacetophenone, kinetics of)
INDEX TERM: 70-11-1
ROLE: PRP (Properties)
(reaction with pyridines, kinetics of)
INDEX TERM: 110-86-1, reactions
ROLE: RCT (Reactant)
(with 2-bromoacetophenone, kinetics of)

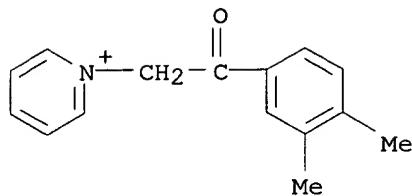
preparation); PREP (Preparation)
 (process for the prepn. of benzothiazolones)
 IT 108773-04-2P
 RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
 (Preparation)
 (process for the prepn. of benzothiazolones)
 IT 55-81-2 532-55-8, Benzoylisothiocyanate
 RL: RCT (Reactant)
 (process for the prepn. of benzothiazolones)

 L17 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 1999 ACS
 AN 1993:495333 HCAPLUS
 DN 119:95333
 TI Preparation of carbazoles as dopaminergic receptor antagonists
 IN Hibino, Satoshi; Okuyama, Shigeru; Nakazato, Atsuo; Kawashima, Yutaka
 PA Taisho Pharma Co Ltd, Japan
 SO Jpn. Kokai Tokkyo Koho, 7 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC ICM C07D209-88
 ICS A61K031-40
 CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 1
 FAN.CNT 1
 PATENT NO. KIND DATE APPLICATION NO. DATE
 ----- ----- ----- -----
 PI JP 05058998 A2 19930309 JP 1991-226856 19910906
 OS MARPAT 119:95333
 GI



I

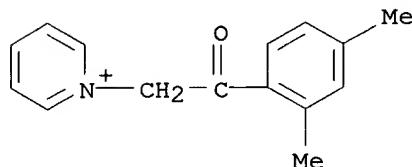
AB Carbazoles I (R1 = H, C1-5 alkyl; R2, R3 = C1-5 alkyl; n = 1-3) and their salts, useful for treatment of aggressive behaviors, excitement, etc., in cerebrovascular disorders and senile dementia, are prepd. Treatment of 0.79 g 1-methoxy-4-(N-propyl-N-propionyl)aminoethylcarbazole (prepn. given) with LiAlH4 in THF at room temp. for 14 h gave 0.71 g I (R1 = Me, R2 = R3 = Et, n = 2) (II), which was converted into HCl salt in 75.4% yield. II inhibited specific binding of (-)-[3H]-sulpiride to adrenergic D2 receptor with IC50 of 648 nM, vs. 86,000 nM, for rimcazole.
 ST adrenergic receptor antagonist carbazole prepn; cerebrovascular disorder dementia treatment carbazole
 IT Adrenergic antagonists
 (carbazoles, for treatment of cerebrovascular disorders and senile dementia)
 IT Mental disorder
 (treatment of, carbazoles for)



● Br⁻

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L6 ANSWER 2 OF 4 REGISTRY COPYRIGHT 1999 ACS
RN 59224-30-5 REGISTRY
CN Pyridinium, 1-[2-(2,4-dimethylphenyl)-2-oxoethyl]-, bromide (9CI)
(CA INDEX NAME)
MF C15 H16 N O . Br
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXLIT
(*File contains numerically searchable property data)



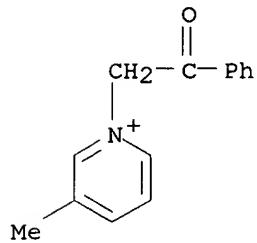
● Br⁻

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L6 ANSWER 3 OF 4 REGISTRY COPYRIGHT 1999 ACS
RN 56567-29-4 REGISTRY
CN Pyridinium, 3,5-dimethyl-1-(2-oxo-2-phenylethyl)-, bromide (9CI)
(CA INDEX NAME)
OTHER NAMES:
CN 3,5-Dimethyl-1-phenacylpyridinium bromide
MF C15 H16 N O . Br
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT
(*File contains numerically searchable property data)
CRN (110854-02-9)



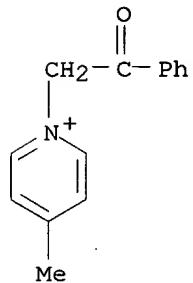
CN 1-Phenacyl-3-picolinium bromide
CN 3-Methyl-1-phenacylpyridinium bromide
MF C14 H14 N O . Br
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, USPATFULL
(*File contains numerically searchable property data)
CRN (59036-97-4)



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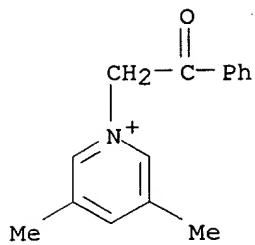
10 REFERENCES IN FILE CA (1967 TO DATE)
10 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L3 ANSWER 4 OF 5 REGISTRY COPYRIGHT 1999 ACS
RN 7250-28-4 REGISTRY
CN Pyridinium, 4-methyl-1-(2-oxo-2-phenylethyl)-, bromide (9CI)
(CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Phenacyl-4-picolinium bromide (6CI)
CN 4-Picolinium, 1-phenacyl-, bromide (8CI)
OTHER NAMES:
CN 1-Phenacyl-4-methylpyridinium bromide
CN 4-Methyl-1-phenacylpyridinium bromide
MF C14 H14 N O . Br
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, IFICDB, IFIPAT,
IFIUDB, TOXLIT, USPATFULL
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CRN (46720-78-9)



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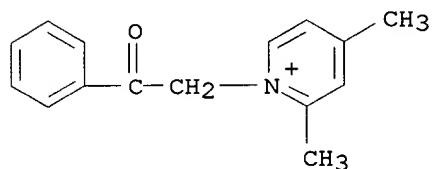
22 REFERENCES IN FILE CA (1967 TO DATE)
22 REFERENCES IN FILE CAPLUS (1967 TO DATE)
1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)



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6 REFERENCES IN FILE CA (1967 TO DATE)
 6 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L6 ANSWER 4 OF 4 REGISTRY COPYRIGHT 1999 ACS
 RN 26557-57-3 REGISTRY
 CN Pyridinium, 2,4-dimethyl-1-(2-oxo-2-phenylethyl)-, bromide (9CI)
 (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN Pyridinium, 2,4-dimethyl-1-phenacyl-, bromide (8CI)
 MF C15 H16 N O . Br
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMINFORMRX
 (*File contains numerically searchable property data)



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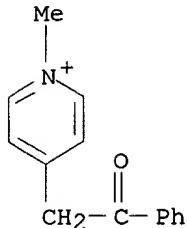
3 REFERENCES IN FILE CA (1967 TO DATE)
 3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> s 56567-29-4/rn
 L7 1 56567-29-4/RN
 => s 16844-10-3/rn
 L8 1 16844-10-3/RN
 => file caplu

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	44.40	44.55

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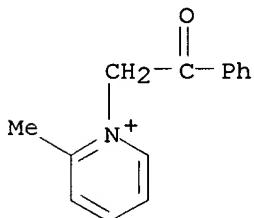
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CRN (188903-44-8)



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1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L3 ANSWER 2 OF 5 REGISTRY COPYRIGHT 1999 ACS
RN 32896-98-3 REGISTRY
CN **Pyridinium, 2-methyl-1-(2-oxo-2-phenylethyl)-, bromide (9CI)**
(CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Picolinium, 1-phenacyl-, bromide (8CI)
OTHER NAMES:
CN **2-Methyl-1-phenacylpyridinium bromide**
CN **2-Methyl-N-phenacylpyridinium bromide**
MF **C14 H14 N O . Br**
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMCATS, CHEMINFORMRX,
CSChem
(*File contains numerically searchable property data)
CRN (136714-42-6)



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18 REFERENCES IN FILE CA (1967 TO DATE)
18 REFERENCES IN FILE CAPLUS (1967 TO DATE)

L3 ANSWER 3 OF 5 REGISTRY COPYRIGHT 1999 ACS
RN 16844-10-3 REGISTRY
CN **Pyridinium, 3-methyl-1-(2-oxo-2-phenylethyl)-, bromide (9CI)**
(CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 3-Picolinium, 1-phenacyl-, bromide (8CI)
OTHER NAMES:
CN **1-Phenacyl-3-methylpyridinium bromide**



IT Cardiovascular system
(disease, treatment of, carbazoles for)

IT Mental disorder
(senile psychosis, treatment of, carbazoles for)

IT 79-03-8, Propionyl chloride
RL: RCT (Reactant)
(amidation of, with methoxyphenethylamine)

IT 55-81-2, 4-Methoxyphenethylamine
RL: RCT (Reactant)
(amidation of, with propionyl chloride)

IT 577-19-5, o-Nitrobromobenzene
RL: RCT (Reactant)
(condensation of, with aminophenethylamine deriv.)

IT 67191-51-9P 102842-44-4P 149081-92-5P **149081-93-6P**
149081-94-7P 149081-95-8P 149081-96-9P 149081-97-0P
149081-98-1P 149081-99-2P 149082-00-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and reaction of)

IT 149060-88-8P 149082-01-9P 149082-02-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, for treatment of cerebrovascular disorders and senile
dementia)

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 13, 1999

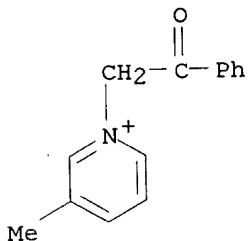
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

=> s 16844-10-3/rn

L1 1 16844-10-3/RN

=> d

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 1999 ACS
 RN 16844-10-3 REGISTRY
 CN Pyridinium, 3-methyl-1-(2-oxo-2-phenylethyl)-, bromide (9CI) (CA INDEX
 NAME)
 OTHER CA INDEX NAMES:
 CN 3-Picolinium, 1-phenacyl-, bromide (8CI)
 OTHER NAMES:
 CN 1-Phenacyl-3-methylpyridinium bromide
 CN 1-Phenacyl-3-picolinium bromide
 CN 3-Methyl-1-phenacylpyridinium bromide
 MF C14 H14 N O . Br
 LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, USPATFULL
 (*File contains numerically searchable property data)
 CRN (59036-97-4)

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10 REFERENCES IN FILE CA (1967 TO DATE)
 10 REFERENCES IN FILE CAPLUS (1967 TO DATE)

=> file caplu

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Et, R = Ph) with NH4OH and refluxing Me2CHOH gave Et 2-phenyl-7-indolizinecarboxylate (IV). Acylation of III and IV by Ac2O, BzCl, and 4-ClC6H4COCl yielded the acylindolizines V (R2 = Me, Ph; R3 = Me, Ph, 4-ClC6H4).

IT 54342-81-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation) (prepn. and cyclization of)

L14 ANSWER 8 OF 8 HCPLUS COPYRIGHT 1999 ACS
AN 1970:77111 HCPLUS

DN 72:77111

TI Further structure-activity relations of heterocyclic analogs of hemicholinium 3

AU Benz, Frederick W.; Long, John Paul

CS Dep. of Pharmacol., Univ. of Iowa, Iowa City, Iowa, USA

SO J. Pharm. Pharmacol. (1970), 22(1), 20-5

CODEN: JPPMAB

DT Journal

LA English

AB The importance of the 3-Me group on the pyridinium ring of bis-quaternary nitrogen salts for hemicholinium-3-like activity having been conditionally established (Benz and Long, 1969), derivs. contg. classical isosteres of the 3-Me group and the 3 oxidn. states of the 3-Me group were examd. Oxidn. of the 3-Me group to CH2OH decreased activity tenfold. Subsequent oxidn. to CHO and CO2H further decreased activity. When the 3-Me group was replaced by a halogen, activity was maintained by the iodo-deriv. but decreased as the size of the halogen decreased and as the electronegativity increased. Substitution of an Et group for the 3-Me decreased activity twofold, whereas replacement with OH eliminated activity.

IT 24620-81-3

RL: BIOL (Biological study)
(neuromuscular inhibition by)